# **Bias-Variance**

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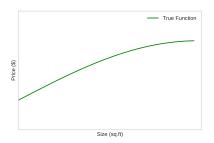
#### The Scenario: True Function

For the purpose of this lecture we assume that there exists a relation between **Housing Prices** and **area of the house**.

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Here, the true function  $f_{\theta_{\text{true}}}$  is used to model the relation  $y_t = f_{\theta_{\text{true}}}(x_t)$ 



Modeling the relation

### The 3 Sources of Error

Any prediction made is affected by 3 sources of error:

Noise

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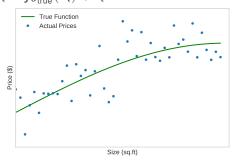
- the condition of the house (cannot be measured perfectly)
- sale prices of other houses in the neighborhood (measurements that have biases in themselves)

Because of this, data is inherently noisy.

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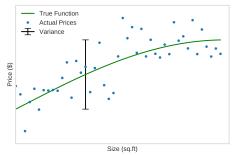
This error can be captured by the error term  $\epsilon$  which causes the final value of the house to follow the equation:  $y_t = f_{\theta_{\text{true}}}(x_t) + \epsilon_t$ 



Modeling the relation

This noise can be assumed to be mean-centered around 0 with spread called the variance of the noise.

This causes  $y_t$  to become mean centered around the true relation.

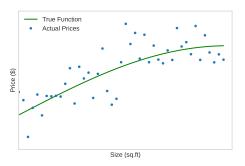


Modeling the relation

**Bias** is a measure of how well a model can fit a given relation.

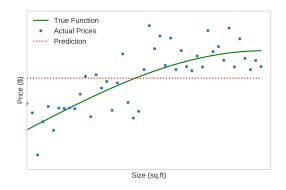
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To understand this, let us take an example where we try to learn the relation that models the *Price* and *Size* of a house using a *constant function*.



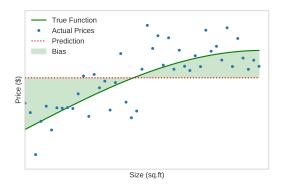
An example dataset

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An example dataset

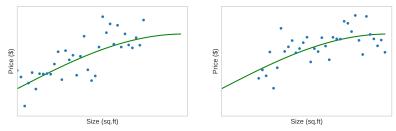
So the bias in this scenario looks something like this:



An example dataset

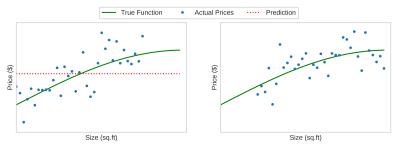
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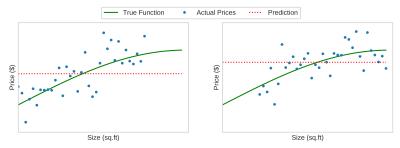
Two Datasets from same relation

But it is important to understand that there are a large number of different datasets possible for a given situation, with each having their individual fits. If we try to fit a constant function to them.



Two Datasets from same relation

But it is important to understand that there are a large number of different datasets possible for a given situation, with each having their individual fits. We see that they show different predictions.



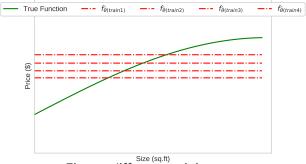
Two Datasets from same relation

#### Doing so for all possible size N training sets we get



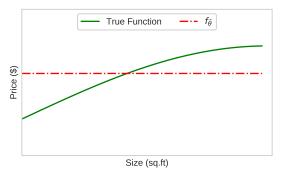
Fits on different training sets

Doing so for all possible size N training sets we get A way of consolidating all these possible fits is to calculate an average fit that is weighted by how likely they are to appear.



Fits on different training sets

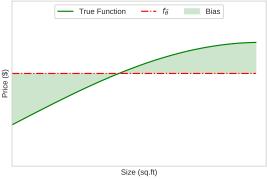
Averaging all the fits (as in this scenario all datasets are equally likely) we get the average fit.



Average fit on all different training sets

### **Bias Contribution**

$$\mathsf{Bias}(\mathsf{x}) = f_{\theta_{\mathsf{true}}}(\mathsf{x}) - f_{\bar{\theta}}(\mathsf{x})$$

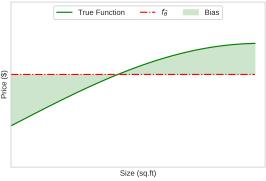


Bias of the fit

#### **Bias Contribution**

$$\mathsf{Bias}(\mathsf{x}) = f_{\theta_{\mathsf{true}}}(\mathsf{x}) - f_{\bar{\theta}}(\mathsf{x})$$

It is a measure of how flexible the fit is in capturing  $f_{\theta_{\mathrm{true}}}(\mathbf{X})$ 

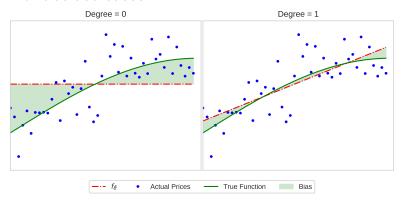


Bias of the fit

# Bias Contribution: Effect of Complexity

As we increase the complexity of the fit

- ⇒ fit becomes more flexible
- ⇒ bias decreases

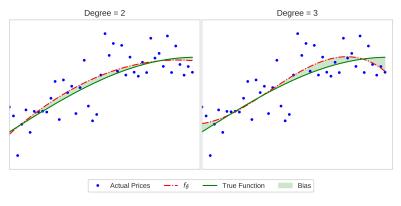


Effect of degree on Bias of the fit

# Bias Contribution: Effect of Complexity

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Effect of degree on Bias of the fit

## Bias: Calculating the Bias

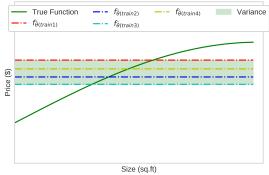
Bias calculation for a model is at the core a calculation of the area under a curve.

Therefore, finding the bias for a model in the range (a,b) is the calculation of the integral:

$$\int_{a}^{b} |f_{\bar{\theta}}(x) - f_{\theta(\mathsf{true})}(x)| dx$$

#### Variance

Variance of the fit is a measure of the variation in the fits when trained across different training sets.

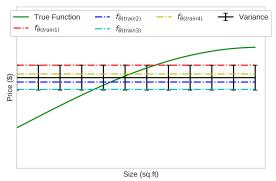


Variance of the fit

#### Variance Contribution

#### For Low Complexity

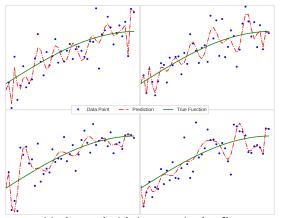
- ⇒ variations between curves are less
- ⇒ Variance is less



Variance of the low complexity fits

### Variance Contribution

#### For High Complexity we see very high variation

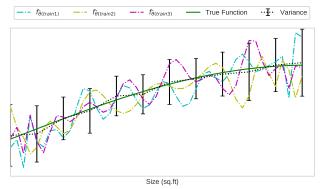


Variance in high complexity fits

#### Variance Contribution

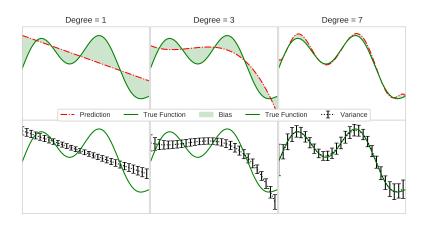
#### For High Complexity

- ⇒ high variation
- ⇒ Variance is high



Variance of the high complexity fits

### The Bias-Variance Trade off



Variance in high complexity fits

#### The Bias-Variance Trade off

Plot Graph - 3:06 Variance and the bias-variance trade off

# Measuring the goodness of a Model

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 $E_{\text{training set}}[\text{error of } \hat{\theta}(\text{training set})]$ 

gives a measure of the average error by doing an expectation of the errors of all possible training sets of size N.

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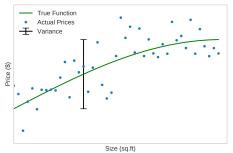
Therefore,  $E_{train}[at a point x_t] = f(noise, bias, variance)$ 

### Formally defining the 3 sources of error: Noise

Noise is an **irreducible error** captured by the error term  $\epsilon$ . The equation of the relation becomes  $y_t = f_{\theta(true)}(x_t) + \epsilon_t$ 

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Variance in the noise

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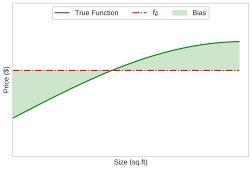
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#### Formally defining the 3 sources of error: Bias

Bias is a measure of how flexible the fit is in capturing the true function  $f_{\theta_{\text{true}}}(x)$ 

$$\mathsf{Bias}(x_t) = f_{\theta_\mathsf{true}}(x_t) - f_{\bar{\theta}}(x_t)$$

where  $f_{ar{ heta}}$  denotes the average fit over all datasets.



Bias of the fit

### Formally defining the 3 sources of error: Bias

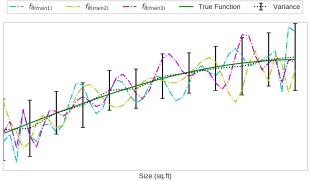
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where  $f_{\bar{\theta}}$  denotes the average fit over all datasets. As  $f_{\bar{\theta}}$  denotes the average fit over all datasets, it can be expressed by  $f_{\bar{\theta}}(x_t) = E_{\text{train}}[f_{\hat{\theta}}(x_t)]$ 

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Variance of a fit

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Variance of the fit is a measure of the variation in the fits when trained across different training sets.

Variance of the fit can be defined by

$$\operatorname{var}(f_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}_t)) = E_{\operatorname{train}}[(f_{\hat{\boldsymbol{\theta}}}(\boldsymbol{x}) - f_{\bar{\boldsymbol{\theta}}}(\boldsymbol{x}_t))^2]$$

where  $f_{\hat{\theta}}(x) - f_{\bar{\theta}}(x_t)$  denotes the deviation that a specific fit has from the average.

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Now we will see how, E_{train}[\text{at a point } x_t] = \sigma^2 + [\text{bias}(f_{\hat{\theta}}(x_t))]^2 + \text{var}(f_{\hat{\theta}}(x_t)) where, given a training set, the parameters \hat{\theta} of the fit are learned as f_{\hat{\theta}} and, the prediction at a point x_t for the model trained on that training set is f_{\hat{\theta}}(x_t)
```

Prediction Error at a point  $x_t$  can be calculated using the squared loss function.

Prediction error at  $x_t = (y_t - f_{\hat{\theta}(train)}(x_t))^2$ 

To find the "Expected Prediction Error" at a point  $x_t$  we average out the prediction error at that point over all possible learned models. This can be done by finding the expectation of prediction error for that point over all possible training datasets (*train*) and labels for that point  $(y_t)$ .

Expected prediction error at  $x_t = E_{train,y_t}[(y_t - f_{\hat{\theta}(train)}(x_t))^2]$ 

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$$= E_{train,y_t}[((y_t - f_{\theta(true)}(x_t)) + (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t)))^2]$$

Expected prediction error at 
$$x_t = E_{train,y_t}[(y_t - f_{\hat{\theta}(train)}(x_t))^2]$$

$$= E_{train,y_t}[(\underbrace{(y_t - f_{\theta(true)}(x_t))}_{a} + \underbrace{(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{b})^2]$$

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$$= E_{train,y_t}[(\alpha + b)^2]$$

Expected prediction error at 
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= 
$$E_{train,y_t}[(a+b)^2]$$

$$= E_{train,y_t}[a^2 + 2ab + b^2]$$

Expected prediction error at 
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(Using Linearity of Expectation) =  $E_{train,y_t}[a^2] + 2E_{train,y_t}[ab] + E_{train,y_t}[b^2]$ ....(Eqn. 1)

$$\textit{E}_{\textit{train},\textit{y}_{\textit{t}}}[\textit{a}^{2}] = \textit{E}_{\textit{train},\textit{y}_{\textit{t}}}[(\textit{y}_{\textit{t}} - \textit{f}_{\textit{\theta}(\textit{true})}(\textit{x}_{\textit{t}}))^{2}]$$

$$\begin{split} E_{train,y_t}[\alpha^2] &= E_{train,y_t}[(y_t - f_{\theta(true)}(x_t))^2] \\ &\qquad \text{(Since there is no dependence on training set)} \\ &= E_{y_t}[(y_t - f_{\theta(true)}(x_t))^2] \end{split}$$

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$$= E_{y_t}[\epsilon_t^2]$$

$$= \sigma^2(\text{By definition})$$

$$E_{train,y_t}[\alpha^2] = \sigma^2......(\text{Eqn. 2})$$

$$\begin{aligned} & \textit{E}_{\textit{train},\textit{y}_t}[\textit{ab}] = \\ & \textit{E}_{\textit{train},\textit{y}_t}[(\textit{y}_t - f_{\theta(\textit{true})}(\textit{x}_t))(f_{\theta(\textit{true})}(\textit{x}_t) - f_{\hat{\theta}(\textit{train})}(\textit{x}_t))] \end{aligned}$$

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$$E_{train,y_t}[b^2] = E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$\begin{split} E_{train,y_t}[b^2] &= E_{train,y_t}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ (f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t) \text{ is independent of } y_t) \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \end{split}$$

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From Eqn. 1, 2, 3 and 4, we get,

Expected prediction error at  $x_t = \sigma^2 + MSE(f_{\hat{\theta}(train)}(x_t))$ 

Now, we will further simplify the MSE term into bias and variance.

$$MSE(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2]$$

$$\begin{split} & \textit{MSE}(f_{\hat{\theta}(\textit{train})}(\textit{x}_t)) = \textit{E}_{\textit{train}}[(f_{\theta(\textit{true})}(\textit{x}_t) - f_{\hat{\theta}(\textit{train})}(\textit{x}_t))^2] \\ \\ & = \textit{E}_{\textit{train}}[((f_{\theta(\textit{true})}(\textit{x}_t) - f_{\bar{\theta}}(\textit{x}_t)) + (f_{\bar{\theta}}(\textit{x}_t) - f_{\hat{\theta}(\textit{train})}(\textit{x}_t)))^2] \end{split}$$

$$\begin{aligned} & \textit{MSE}(f_{\hat{\theta}(\textit{train})}(\textit{x}_t)) = \textit{E}_{\textit{train}}[(f_{\theta(\textit{true})}(\textit{x}_t) - f_{\hat{\theta}(\textit{train})}(\textit{x}_t))^2] \\ & = \textit{E}_{\textit{train}}[(\underbrace{(f_{\theta(\textit{true})}(\textit{x}_t) - f_{\bar{\theta}}(\textit{x}_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(\textit{x}_t) - f_{\hat{\theta}(\textit{train})}(\textit{x}_t))}_{\beta})^2] \end{aligned}$$

$$\begin{split} & \textit{MSE}(f_{\hat{\theta}(\textit{train})}(\textit{X}_t)) = \textit{E}_{\textit{train}}[(f_{\theta(\textit{true})}(\textit{X}_t) - f_{\hat{\theta}(\textit{train})}(\textit{X}_t))^2] \\ & = \textit{E}_{\textit{train}}[(\underbrace{(f_{\theta(\textit{true})}(\textit{X}_t) - f_{\bar{\theta}}(\textit{X}_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(\textit{X}_t) - f_{\hat{\theta}(\textit{train})}(\textit{X}_t)))^2}_{\beta}] \\ & = \textit{E}_{\textit{train}}[(\alpha + \beta)^2] \end{split}$$

$$\begin{split} & \textit{MSE}(f_{\hat{\theta}(\textit{train})}(x_t)) = \textit{E}_{\textit{train}}[(f_{\theta(\textit{true})}(x_t) - f_{\hat{\theta}(\textit{train})}(x_t))^2] \\ & = \textit{E}_{\textit{train}}[(\underbrace{(f_{\theta(\textit{true})}(x_t) - f_{\bar{\theta}}(x_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(\textit{train})}(x_t))}_{\beta})^2] \\ & = \textit{E}_{\textit{train}}[(\alpha + \beta)^2] \\ & = \textit{E}_{\textit{train}}[\alpha^2 + 2\alpha\beta + \beta^2] \end{split}$$

$$\begin{split} & \mathit{MSE}(f_{\hat{\theta}(train)}(x_t)) = E_{train}[(f_{\theta(true)}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(\underbrace{(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))}_{\alpha} + \underbrace{(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))}_{\beta})^2] \\ &= E_{train}[(\alpha + \beta)^2] \\ &= E_{train}[\alpha^2 + 2\alpha\beta + \beta^2] \\ & ( \mathsf{Using Linearity of Expectation} ) \\ &= E_{train}[\alpha^2] + 2E_{train}[\alpha\beta] + E_{train}[\beta^2] \dots (\mathsf{Eqn. 5}) \end{split}$$

$$E_{train}[\alpha^2] = E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2]$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \end{split}$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \\ &= E_{train}[bias(f_{\hat{\theta}}(x_t))^2] \end{split} \tag{By definition of bias)}$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \\ &= E_{train}[bias(f_{\hat{\theta}}(x_t))^2] \qquad \text{(By definition of bias)} \\ &= bias(f_{\hat{\theta}}(x_t))^2 \\ &\text{($\cdots$ bias is not a function of training data)} \end{split}$$

$$\begin{split} E_{train}[\alpha^2] &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\theta(true)}(x_t) - E_{train}[f_{\hat{\theta}(train)}(x_t)]^2] \\ &= E_{train}[bias(f_{\hat{\theta}}(x_t))^2] \qquad \text{(By definition of bias)} \\ &= bias(f_{\hat{\theta}}(x_t))^2 \\ &\text{($\because$ bias is not a function of training data)} \\ E_{train}[\alpha^2] &= bias(f_{\hat{\theta}}(x_t))^2 \dots (Eqn. 6) \end{split}$$

$$\begin{aligned} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \end{aligned}$$

$$\begin{split} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train}[bias_t \times (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta]\\ &=E_{train}[(f_{\theta(true)}(x_t)-f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t))]\\ &=E_{train}[bias_t\times(f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t))]\\ &=bias_t\times E_{train}[f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t)]\\ &(\because bias_t \text{ is not a function of training data}) \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta] \\ &= E_{train}[(f_{\theta(true)}(x_t) - f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= E_{train}[bias_t \times (f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))] \\ &= bias_t \times E_{train}[f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t)] \\ &(\because bias_t \text{ is not a function of training data}) \\ &= bias \times \left(E_{train}[f_{\bar{\theta}}(x_t)] - E_{train}[f_{\hat{\theta}(train)}(x_t)]\right) \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta]\\ &=E_{train}[(f_{\theta(true)}(x_t)-f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t))]\\ &=E_{train}[bias_t\times(f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t))]\\ &=bias_t\times E_{train}[f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t)]\\ &(\because bias_t \text{ is not a function of training data})\\ &=bias\times\left(E_{train}[f_{\bar{\theta}}(x_t)]-E_{train}[f_{\hat{\theta}(train)}(x_t)]\right)\\ &=bias\times(f_{\bar{\theta}}(x_t)-f_{\bar{\theta}}(x_t))\\ &(\because f_{\bar{\theta}}(x_t)=E_{train}[f_{\hat{\theta}(train)}(x_t)]) \end{split}$$

$$\begin{split} &E_{train}[\alpha\beta]\\ &=E_{train}[(f_{\theta(true)}(x_t)-f_{\bar{\theta}}(x_t))(f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t))]\\ &=E_{train}[bias_t\times(f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t))]\\ &=bias_t\times E_{train}[f_{\bar{\theta}}(x_t)-f_{\hat{\theta}(train)}(x_t)]\\ &(\because bias_t \text{ is not a function of training data})\\ &=bias\times\left(E_{train}[f_{\bar{\theta}}(x_t)]-E_{train}[f_{\hat{\theta}(train)}(x_t)]\right)\\ &=bias\times(f_{\bar{\theta}}(x_t)-f_{\bar{\theta}}(x_t))\\ &E_{train}[\alpha\beta]=0......(Eqn. 7) \end{split}$$

$$E_{train}[\beta^2] = E_{train}[(f_{\bar{\theta}}(\mathbf{x}_t) - f_{\hat{\theta}(train)}(\mathbf{x}_t))^2]$$

$$\begin{aligned} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(\mathbf{x}_t) - f_{\hat{\theta}(train)}(\mathbf{x}_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(\mathbf{x}_t) - f_{\bar{\theta}}(\mathbf{x}_t))^2] \end{aligned}$$

$$\begin{split} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - E_{train}[(f_{\hat{\theta}(train)}(x_t))^2] \\ & \\ & (\because f_{\bar{\theta}}(x_t) = E_{train}[(f_{\hat{\theta}(train)}(x_t))] \ ) \end{split}$$

$$\begin{split} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - E_{train}[(f_{\hat{\theta}(train)}(x_t)])^2] \\ & (\because f_{\bar{\theta}}(x_t) = E_{train}[(f_{\hat{\theta}(train)}(x_t)]) \\ &= variance(f_{\hat{\theta}}(x_t)) \end{split}$$

$$\begin{split} E_{train}[\beta^2] &= E_{train}[(f_{\bar{\theta}}(x_t) - f_{\hat{\theta}(train)}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - f_{\bar{\theta}}(x_t))^2] \\ &= E_{train}[(f_{\hat{\theta}(train)}(x_t) - E_{train}[(f_{\hat{\theta}(train)}(x_t)])^2] \\ & (\because f_{\bar{\theta}}(x_t) = E_{train}[(f_{\hat{\theta}(train)}(x_t)]) \\ &= variance(f_{\hat{\theta}}(x_t)) \\ E_{train}[\beta^2] &= variance(f_{\hat{\theta}}(x_t))...................(Eqn. 8) \end{split}$$

From Eqn. 1 - 8, we get,

Expected prediction error at  $x_t$ 

$$=\sigma^2 + MSE(f_{\hat{\theta}(train)}(x_t))$$

$$= \sigma^2 + \textit{bias}(f_{\hat{\theta}}(\textit{x}_{\textit{t}}))^2 + \textit{variance}(f_{\hat{\theta}}(\textit{x}_{\textit{t}}))$$